Supplementary Data: Details of Predictions located during post-analysis

Table S3. Lattice parameter deviations, Δ*E* and RMSD for the experimental and predicted structures of molecule XVI. α = β = γ = 90° in all structures.

	Rank	Δ*E* [a] (kJ/mol)	density (g/cm^3)	*a* (Å)	*b* (Å)	*c* (Å)	$RMSD_{15}$ [b] (Å)
expt. (*T* = 174 K)	-	-	1.385	9.645(2)	7.381(1)	16.185(3)	-
not located in search, but energy minimised in post-analysis							
Hofmann	-	+1.51	-2.5%	+2.5%	+0.6%	-0.6%	0.115
Misquitta, Pickard, Needs	-	-0.05[c]	+5.6%	-0.4%	-3.9%	-1.1%	0.145
Scheraga, Arnautova	-	+2.59	-5.9%	+1.6%	+3.9%	+0.6%	0.224

[a] Δ*E* is calculated with respect to the lowest energy structure predicted by the same research group.
[b] $RMSD_{15}$ is calculated using a 15 molecule comparison in the Materials Module of Mercury, ignoring H atoms.
[c] Δ*E* for the global minimum is calculated with respect to the second lowest energy structure.

Table S4. Lattice parameter deviations, Δ*E* and $RMSD_{15}$ for the experimental and predicted structures of molecule XVII. α = γ = 90° in all structures.

	Rank	Δ*E* [a] (kJ/mol)	density (g/cm^3)	*a* (Å)	*b* (Å)	*c* (Å)	β (°)	$RMSD_{15}$ [b] (Å)
expt. (*T* = 174 K)	-	-	1.837	12.639(1)	5.979(1)	11.422(1)	96.807(1)	-
not located in search, but energy minimised in post-analysis								
Hofmann	-	+2.75	-1.8%	+0.9%	-0.6%	+1.8%	+2.8%	0.229
Scheraga, Arnautova	-	+5.34	-2.6%	+2.1%	0.0%	+0.2%	+0.6%	0.193

[a] Δ*E* is calculated with respect to the lowest energy structure predicted by the same research group.
[b] $RMSD_{15}$ is calculated using a 15 molecule comparison in the Materials Module of Mercury, ignoring H atoms.

Table S5. Lattice parameter deviations, Δ*E* and RMSD for the experimental and predicted structures of molecule XVIII. α = β = γ = 90° in all structures.

	Rank	Δ*E* [a] (kJ/mol)	density (g/cm^3)	*a* (Å)	*b* (Å)	*c* (Å)	$RMSD_{15}$ [b] (Å)
expt. (*T* = 174 K)	-	-	1.566	9.889(1)	8.887(1)	24.969(3)	-
not located in search, but energy minimised in post-analysis							
Hofmann	-	+2.56	-1.6%	+1.6%	+0.2%	+0.2%	0.135
Price, Price	-	+5.03	-2.9%	+0.7%	+1.9%	0.0%	0.100
Boerrigter	-	-0.58 [c]	+0.3%	+1.7%	+0.5%	-2.0%	0.439

Van Eijck	-	+29.30	-1.7%	+0.8%	+2.4%	-0.3%	0.188

[a] Δ*E* is calculated with respect to the lowest energy structure predicted by the same research group.
[b] $RMSD_{15}$ is calculated using a 15 molecule comparison in the Materials Module of Mercury, ignoring H atoms.
[c] Δ*E* for the global minimum is calculated with respect to the second lowest energy structure.

Table S6. Lattice parameter deviations, Δ*E* and RMSD for the experimental and predicted structures of molecular salt XIX. α = β = γ = 90° in all structures.

	Rank	Δ*E* [a] (kJ/mol)	density (g/cm^3)	*a* (Å)	*b* (Å)	*c* (Å)	$RMSD_{15}$ [b] (Å)
expt. (*T* = 200 K)	-	-	1.481	23.501(3)	3.714(1)	12.654(1)	-
not located in search, but energy minimised in post-analysis							
Hofmann	-	+12.43	-7.3%	+6.0%	+0.3%	+0.7%	0.301
Price, Mohamed	-	+10.21	-3.2%	-2.2%	+2.0%	+3.7%	0.265
Scheraga, Arnautova	-	+0.32	-1.4%	-2.4%	-1.2%	+5.1%	0.542

[a] Δ*E* is calculated with respect to the lowest energy structure predicted by the same research group.
[b] $RMSD_{15}$ is calculated using a 15 molecule comparison in the Materials Module of Mercury, ignoring H atoms.

Table S7. Lattice parameter deviations, Δ*E* and $RMSD_{15}$ for the experimental and predicted structures of molecule XX. α = γ = 90° in all structures.

	Rank	Δ*E* [a] (kJ/mol)	density (g/cm^3)	*a* (Å)	*b* (Å)	*c* (Å)	β (°)	$RMSD_{15}$ [b] (Å)
expt. (*T* = 150 K)	-	-	1.411	14.078(1)	6.356(1)	25.310(2)	96.063(2)	-
not located in search, but energy minimised in post-analysis								
Hofmann	-	+2.43	+0.4%	+1.0%	-2.1%	+0.9%	+1.3%	0.297
Van Eijck	-	-11.40[c]	-0.8%	+1.4%	-2.5%	+2.6%	+4.1%	0.435

[a] Δ*E* is calculated with respect to the lowest energy structure predicted by the same research group.
[b] $RMSD_{15}$ is calculated using a 15 molecule comparison in the Materials Module of Mercury, ignoring H atoms.
[c] Δ*E* for the global minimum is calculated with respect to the second lowest energy structure.

Table S8a. Lattice parameter deviations, Δ*E* and $RMSD_{15}$ for the experimental and predicted structures of hydrate XXI (with matching hydrogen placement). α = γ = 90° in all structures.

	Rank	Δ*E* [a] (kJ/mol)	density (g/cm^3)	*a* (Å)	*b* (Å)	*c* (Å)	β (°)	$RMSD_{15}$ [b] (Å)
expt. (*T* = 150 K)	-	-	1.639	9.790(7)	3.609(3)	21.583(16)	91.462(14)	-
not located in search, but energy minimised in post-analysis								
Hofmann	-	+2.10	+1.9%	+1.3%	-1.5%	+2.7%	+2.7%	0.159

[a] Δ*E* is calculated with respect to the lowest energy structure predicted by the same research group.
[b] $RMSD_{15}$ is calculated using a 15 molecule comparison in the Materials Module of Mercury, ignoring H atoms.

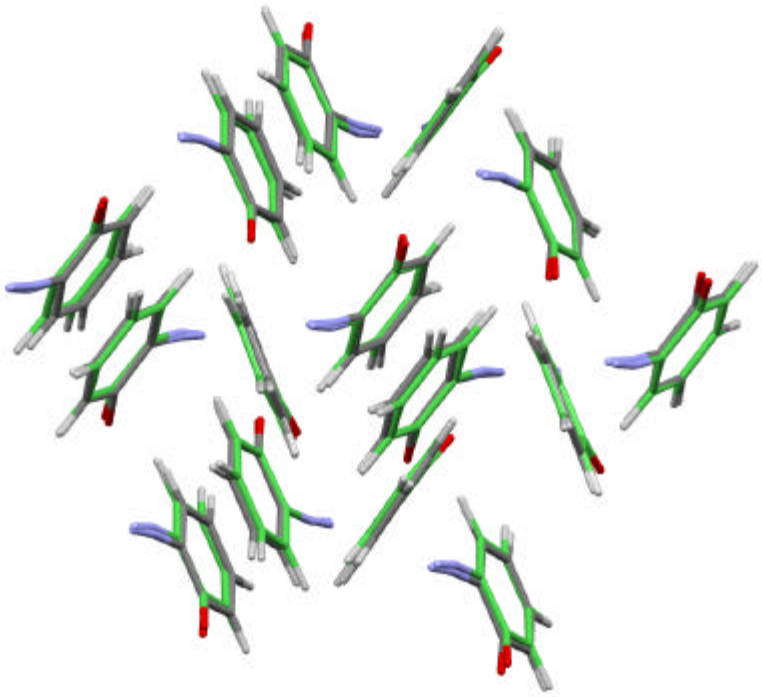

Figure S1. Overlay of the unit-cell contents of the observed crystal structure XVI (green) and Neumann *et al.* XVI.1 (grey). $RMSD_{15}$ 0.157 Å

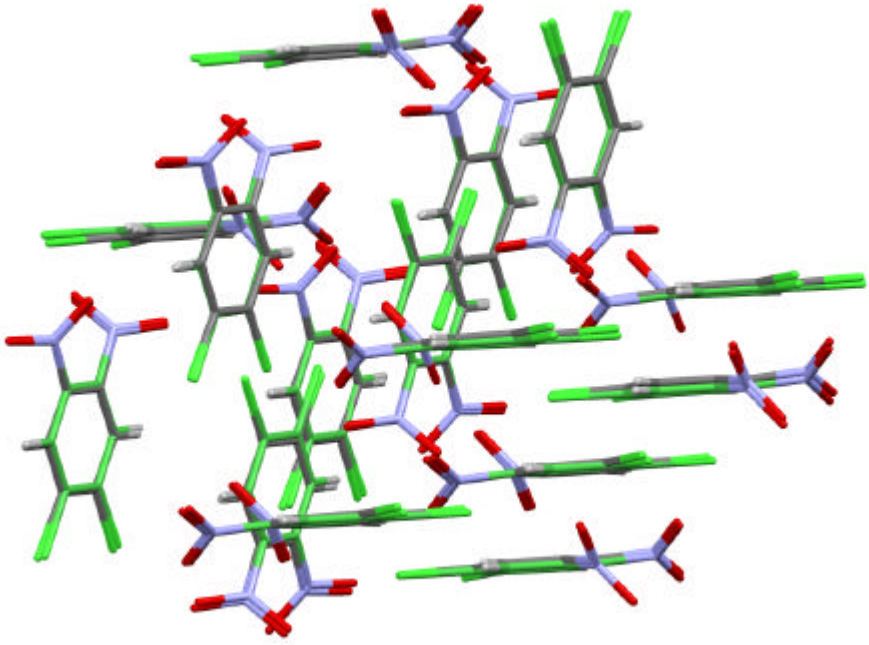

Figure S2. Overlay of the unit-cell contents of the observed crystal structure XVII (green) and Price *et al.* XVII.2 (grey). $RMSD_{15}$ 0.130 Å

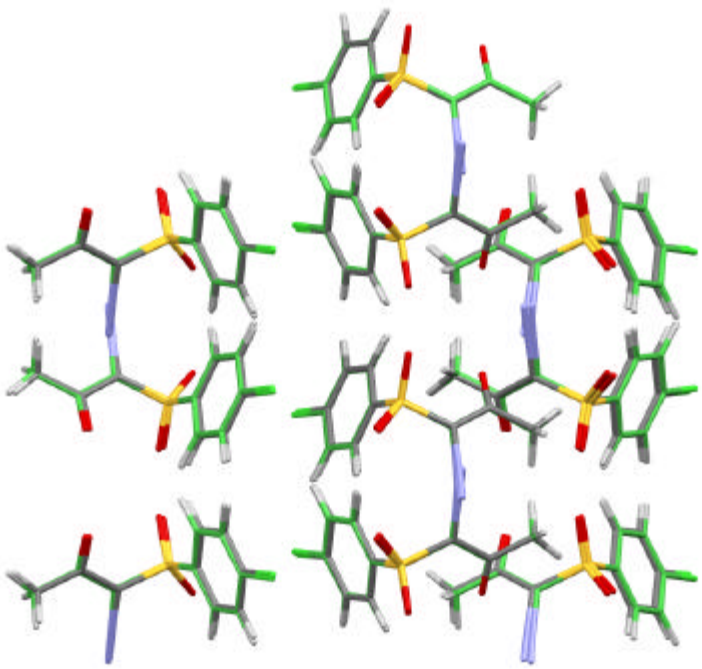

Figure S3. Overlay of the unit-cell contents of the observed crystal structure XVIII (green) and Neumann *et al.* XVIII.1 (grey). RMSD 0.122 Å

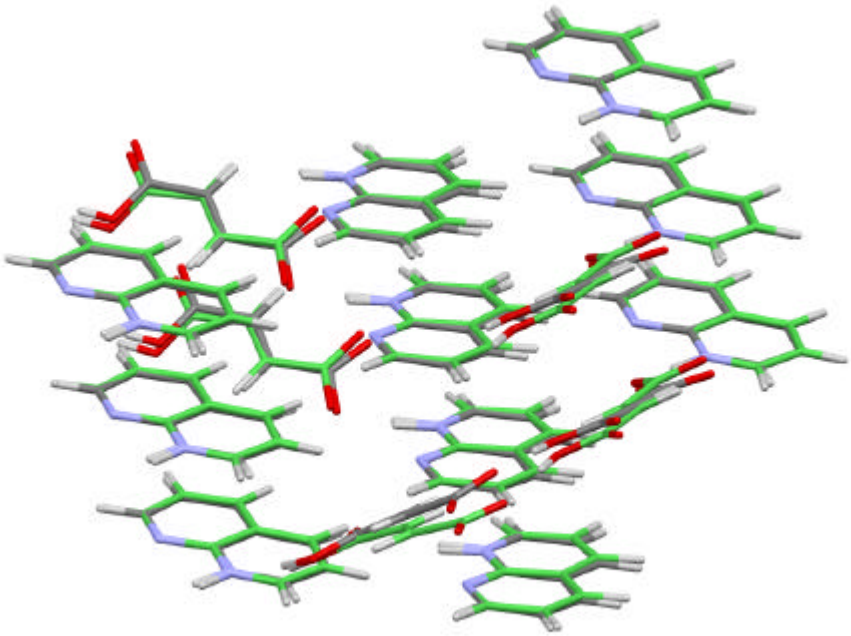

Figure S4. Overlay of the unit-cell contents of the observed crystal structure XIX (green) and van Eijck XIX.2 (grey). RMSD 0.220 Å

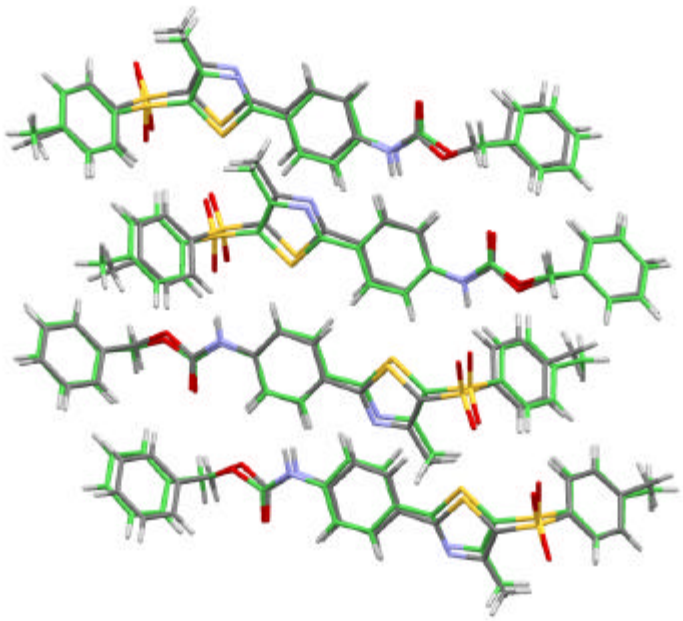

Figure S5. Overlay of the unit-cell contents of the observed crystal structure XX (green) and Day *et al.* XX.1 (grey). RMSD 0.429 Å